Upper Bound for the Coefficients of Chromatic polynomials

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Abstract

This paper describes an improvement in the upper bound for the magnitude of a coefficient of a term in the chromatic polynomial of a general graph. If a_r is the coefficient of the q^r term in the chromatic polynomial $P(G,q)$, where q is the number of colors, then we find $a_r \le \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-k_g-g+2}{v-r-g+2} - \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \binom{e-g+1-n-m}{v-r-g} - \delta_{g,3} \sum_{n=1}^{k_g+\ell^*_{g+1}-\ell_g} \binom{e-\ell_g-g+1-n}{v-r-g}$, where k_g is the number of circuits of length g and ℓ_g and ℓ^*_{g+1} are certain numbers defined in the text.

key words: chromatic polynomial

1 Introduction

Let G be a loopless graph with v vertices and e edges. The chromatic polynomial $P(G,q)$ counts the number of ways of coloring the vertices of G with q colors subject to the condition that adjacent vertices have different colors [1, 2]. (More generally, one may consider multi-graphs G with multiple edges; however, it is elementary that the chromatic polynomial for a graph with multiple edges joining two vertices v and v' is the same as for the graph with just one edge joining these vertices.) Besides its role in graph theory, this polynomial is of interest in statistical physics as the zero-temperature value of a certain model of cooperative phenomena and phase transitions known as the Potts model (e.g., [5, 13] and references therein.). The chromatic polynomial of a graph can be calculated by means of the iterative use of the deletion-contraction theorem or equivalently, the addition-contraction theorem, which explicitly shows that it is a polynomial of maximal degree v in q. It can be written as

$$P(G,q) = \sum_{r=1}^{v} (-1)^{v-r} a_r q^r \ . \tag{1.1}$$

Since the chromatic polynomial of a set of graphs is the product of the chromatic polynomials of each individual graph, we shall restrict our attention to a connected graph.

2 Basic Properties of a_r

Since the calculation of $P(G,q)$ is, in general, a #P-hard problem [11]), it is useful to have bounds on the coefficients. The coefficients of a chromatic polynomial can be expressed as the sum of the number of its subgraphs which do not contain any broken circuit [4, 8].

By an elementary application of the deletion-contraction theorem, it follows that the coefficients a_r in eq. (1.1) are positive. Furthermore, the leading terms are [7]

$$a_r = \begin{cases} \binom{e}{v-r} & \text{if} \quad r > v-g+1 \\ \binom{e}{v-r} - k_g & \text{if} \quad r = v-g+1 \end{cases} \tag{2.1}$$

where g is the girth of the graph, and k_g is the number of circuits of length g in the graph. In particular, $a_v = 1$ and $a_{v-1} = e$.

In practice, one finds that the a_r increase monotonically as r decreases from v, with at most two of these coefficients having the maximal value, and then the a_r decrease monotonically for lower values of r. We can easily show that the magnitude of a_j can not just increase monotonically without decreasing as follows,

Proposition 1 The statement that $a_r \le a_{r-1} \quad \forall\ 1 \le r \le v$ is false except for the trivial case $e = 1$.

Proof This statement is equivalent to

$$a_v \le a_{v-1} \le a_{v-2} \le ... \le a_1 \ . \tag{2.2}$$

Here we consider the graph with $e \ge 2$, and therefore, *a fortiori*, $P(G, q = 1) = 0$. However, eq. (2.2) implies

$$\begin{aligned} P(G, q = 1) &= a_v - a_{v-1} + a_{v-2} - a_{v-3} + ... + (-1)^{v-1} a_1 \\ &= 1 - e + a_{v-2} - a_{v-3} + ... + (-1)^{v-1} a_1 \neq 0 \ . \end{aligned} \tag{2.3}$$

This contradiction disproves the statement except for the trivial case: the tree graph with only two vertices and one edge has $P(T_2, q) = q(q-1) = q^2 - q$. □

Recall the deletion-contraction theorem [2]-[1]: Let x and y be adjacent vertices in G, and denote the edge joining them as xy. Then

$$P(G, q) = P(G - xy, q) - P(G/xy, q) \tag{2.4}$$

where $G - xy$ is the graph obtained from G by deleting the edge xy, and G/xy is the graph obtained from G by deleting the edge xy and identifying x and y.

If we also write

$$P(G - xy, q) = \sum_{r=1}^{v} (-1)^{v-r} a'_r q^r \tag{2.5}$$

and

$$P(G/xy, q) = \sum_{r=1}^{v-1} (-1)^{v-1-r} a''_r q^r , \tag{2.6}$$

then

$$a_r = a'_r + a''_r \quad \text{for} \quad 1 \le r \le v - 1 \ . \tag{2.7}$$

3 Upper Bound on a_r

It was known that the coefficients a_r's are bounded above by the corresponding coefficients of the complete graph with the same number of vertices, K_v [8]. However, this upper bound is sharp only for complete graphs.

An upper bound on a_r was given by Li and Tian [6] and is

$$a_r \le \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-k_g-g+2}{v-r-g+2} \ . \tag{3.1}$$

We improve this bound. Let us use the convention

$$\binom{a}{b} = \begin{cases} 1 & \text{if} \quad b = 0 \\ 0 & \text{if} \quad b > a \text{ or } b < 0 \end{cases} \tag{3.2}$$

and, for some function $f(n)$

$$\sum_{n=0}^{m} f(n) = 0 \quad \text{if} \quad m < 0 \ . \tag{3.3}$$

Therefore, the bound reduced to the exact values in eq. (2.1) when $r \geq v - g + 1$.

Let us derive a basic relation which will be used repeatedly later:

Lemma 1 If $a > b \geq c \geq 0$, then

$$-\binom{a}{c} + \binom{b}{c} = -\sum_{n=1}^{a-b} \binom{a-n}{c-1} \ . \tag{3.4}$$

Proof We know

$$\begin{aligned} \binom{b+1}{c} - \binom{b}{c-1} &= \frac{(b+1)!}{c!(b+1-c)!} - \frac{b!}{(c-1)!(b-c+1)!} \\ &= \frac{b!}{(c-1)!(b+1-c)!}\left[\frac{b+1}{c} - 1\right] \\ &= \frac{b!}{(c-1)!(b+1-c)!}\frac{b+1-c}{c} \\ &= \frac{b!}{c!(b-c)!} \\ &= \binom{b}{c}, \end{aligned} \tag{3.5}$$

and the result follows if we keep on applying this relation on the positive term generated from $\binom{b}{c}$. □

Next we prove a lemma that will be used for our bound. To begin, we make a choice of a certain edge xy in G where we shall apply the deletion-contraction theorem. We then define ℓ_g as the number of circuits in G of length g that contain this edge xy.

Lemma 2 If the number of circuits of length n in a graph G is k_n, where $k_n \geq 0$, $g \leq n \leq s$, $g \leq s \leq v$, and the number of circuits of length n containing the edge xy is ℓ_n, then there are v vertices and $e - 1$ edges in graph $G - xy$, and the number of circuits of length n is $k'_n = k_n - \ell_n$. For the graph G/xy, there are $v - 1$ vertices, and the number of edges and the number of circuits of length n are (i) $e - 1$ and $k''_n = k_n - \ell_n + \ell_{n+1}$ if $\ell_3 = 0$,

or (ii) $e-\ell_3-1$ and $k''_n = k_n - \ell_n + \ell^*_{n+1}$ if $\ell_3 \neq 0$, where ℓ^*_{n+1} is the number of circuits of length $n+1$ which do not contain the edge xz (or the edge yz) for any vertex z.

Proof The number of vertices and edges is clear for $G-xy$, and G/xy when $\ell_3 = 0$. If $\ell_3 \neq 0$, the contraction of the edge xy will result in ℓ_3 double edges, and one of these edges can be removed from each pair without affecting the chromatic polynomial. The circuits of length $n+1$ in G which become the circuits of length n in G/xy and contain both edges xy and xz (or yz) are double-counted. They are the same as the circuits of length n in G which contain the edge yz (or xz) but not the edge xy. $\square$

Now the upper bound of Li and Tian can be improved with extra negative terms.

Theorem 1 If the girth of a graph G is g, and the number of circuits of length g in the graph is k_g, then

$$\begin{aligned} a_r \leq & \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-k_g-g+2}{v-r-g+2} \\ & - \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \binom{e-g+1-n-m}{v-r-g} - \delta_{g,3} \sum_{n=1}^{k_g+\ell^*_{g+1}-\ell_g} \binom{e-\ell_g-g+1-n}{v-r-g}, \end{aligned} \tag{3.6}$$

where, as defined above, ℓ_g and ℓ^*_{g+1} are determined by the initial choice of the edge xy on which we apply the deletion-contraction theorem.

Proof Consider the special case $g=3$ first. By eq. (3.1) and Lemma 2

$$\begin{aligned} a'_r &\leq \binom{e-1}{v-r} - \binom{(e-1)-3+2}{v-r-3+2} + \binom{(e-1)-(k_3-\ell_3)-3+2}{v-r-3+2} \\ &= \binom{e-1}{v-r} - \binom{e-2}{v-r-1} + \binom{e-2-k_3+\ell_3}{v-r-1} \end{aligned} \tag{3.7}$$

$$\begin{aligned} a''_r &\leq \binom{e-\ell_3-1}{(v-1)-r} - \binom{(e-\ell_3-1)-3+2}{(v-1)-r-3+2} + \binom{(e-\ell_3-1)-(k_3-\ell_3+\ell^*_4)-3+2}{(v-1)-r-3+2} \\ &= \binom{e-\ell_3-1}{v-r-1} - \binom{e-\ell_3-2}{v-r-2} + \binom{e-k_3-\ell^*_4-2}{v-r-2} \end{aligned} \tag{3.8}$$

then by eq. (2.7) and Lemma 1,

$$\begin{aligned} a_r \leq & \binom{e-1}{v-r} - \binom{e-2}{v-r-1} + \binom{e-2-k_3+\ell_3}{v-r-1} \\ & + \binom{e-\ell_3-1}{v-r-1} - \binom{e-\ell_3-2}{v-r-2} + \binom{e-k_3-\ell^*_4-2}{v-r-2} \end{aligned}$$

$$\begin{aligned}
&= \binom{e}{v-r} - \binom{e-1}{v-r-1} - \sum_{n=1}^{k_3-\ell_3}\binom{e-2-n}{v-r-2} + \binom{e-\ell_3-1}{v-r-1} \\
&\quad -\binom{e-k_3-1}{v-r-1} + \binom{e-k_3-1}{v-r-1} - \sum_{n=1}^{k_3+\ell_4^*-\ell_3}\binom{e-\ell_3-2-n}{v-r-3} \\
&= \binom{e}{v-r} - \binom{e-1}{v-r-1} + \binom{e-k_3-1}{v-r-1} - \sum_{n=1}^{k_3-\ell_3}\binom{e-2-n}{v-r-2} \\
&\quad +\sum_{n=1}^{k_3-\ell_3}\binom{e-\ell_3-1-n}{v-r-2} - \sum_{n=1}^{k_3+\ell_4^*-\ell_3}\binom{e-\ell_3-2-n}{v-r-3} \\
&= \binom{e}{v-r} - \binom{e-1}{v-r-1} + \binom{e-k_3-1}{v-r-1} \\
&\quad -\sum_{n=1}^{k_3-\ell_3}\sum_{m=1}^{\ell_3-1}\binom{e-2-n-m}{v-r-3} - \sum_{n=1}^{k_3+\ell_4^*-\ell_3}\binom{e-\ell_3-2-n}{v-r-3}\,. \qquad (3.9)
\end{aligned}$$

Consider $g > 3$ and choose the edge xy so that the girth of G/xy is $g-1$ and the number of circuits of length $g-1$ is ℓ_g. By eq. (3.1) and Lemma 2

$$\begin{aligned}
a'_r &\leq \binom{e-1}{v-r} - \binom{(e-1)-g+2}{v-r-g+2} + \binom{(e-1)-(k_g-\ell_g)-g+2}{v-r-g+2} \\
&= \binom{e-1}{v-r} - \binom{e-g+1}{v-r-g+2} + \binom{e-k_g+\ell_g-g+1}{v-r-g+2} \qquad (3.10)
\end{aligned}$$

$$\begin{aligned}
a''_r &\leq \binom{e-1}{(v-1)-r} - \binom{(e-1)-(g-1)+2}{(v-1)-r-(g-1)+2} + \binom{(e-1)-\ell_g-(g-1)+2}{(v-1)-r-(g-1)+2} \\
&= \binom{e-1}{v-r-1} - \binom{e-g+2}{v-r-g+2} + \binom{e-\ell_g-g+2}{v-r-g+2} \qquad (3.11)
\end{aligned}$$

therefore,

$$\begin{aligned}
a_r &\leq \binom{e-1}{v-r} - \binom{e-g+1}{v-r-g+2} + \binom{e-k_g+\ell_g-g+1}{v-r-g+2} \\
&\quad +\binom{e-1}{v-r-1} - \binom{e-g+2}{v-r-g+2} + \binom{e-\ell_g-g+2}{v-r-g+2} \\
&= \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} - \sum_{n=1}^{k_g-\ell_g}\binom{e-g+1-n}{v-r-g+1} \\
&\quad +\binom{e-k_g-g+2}{v-r-g+2} - \binom{e-k_g-g+2}{v-r-g+2} + \binom{e-\ell_g-g+2}{v-r-g+2}
\end{aligned}$$

$$
\begin{aligned}
&= \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-k_g-g+2}{v-r-g+2} \\
&\quad - \sum_{n=1}^{k_g-\ell_g} \binom{e-g+1-n}{v-r-g+1} + \sum_{n=1}^{k_g-\ell_g} \binom{e-\ell_g-g+2-n}{v-r-g+1} \\
&= \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-k_g-g+2}{v-r-g+2} \\
&\quad - \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \binom{e-g+1-n-m}{v-r-g} \ .
\end{aligned} \tag{3.12}
$$

□

It is obvious that this bound of a_r is reduced to the Li-Tian bound in eq. (3.1) when $k_g = \ell_g = 1$, and is optimized if we choose the edge xy so that the magnitude of the summation S, where

$$
S = \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \binom{e-g+1-n-m}{v-r-g} \tag{3.13}
$$

is as large as possible. By Lemma 1, we can rewrite the bound as

$$
\begin{aligned}
a_r \ \leq \ & \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-\ell_g-g+2}{v-r-g+2} - \binom{e-g+1}{v-r-g+2} \\
& + \binom{e-k_g+\ell_g-g+1}{v-r-g+2} - \delta_{g,3}\Big[\binom{e-\ell_g-g+1}{v-r-g+1} \\
& - \binom{e-k_g-\ell^*_{g+1}-g+1}{v-r-g+1}\Big] \ .
\end{aligned} \tag{3.14}
$$

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